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APPLICATION NO.	FILING DATE	FIRST NAMED INVENTOR	ATTORNEY DOCKET NO.	CONFIRMATION NO.
10/723,594	11/26/2003	Yuan-Ping Pang	07039-161002	7578

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EXAMINER

NEGIN, RUSSELL SCOTT

ART UNIT	PAPER NUMBER
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1631

DATE MAILED: 12/27/2005

Please find below and/or attached an Office communication concerning this application or proceeding.

**Office Action Summary**

Application No.

10/723,594

Applicant(s)

PANG, YUAN-PING

Examiner

Russell S. Negin

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-- The MAILING DATE of this communication appears on the cover sheet with the correspondence address --

**Period for Reply**

A SHORTENED STATUTORY PERIOD FOR REPLY IS SET TO EXPIRE 1 MONTH(S) OR THIRTY (30) DAYS, WHICHEVER IS LONGER, FROM THE MAILING DATE OF THIS COMMUNICATION.

- Extensions of time may be available under the provisions of 37 CFR 1.136(a). In no event, however, may a reply be timely filed after SIX (6) MONTHS from the mailing date of this communication.
- If NO period for reply is specified above, the maximum statutory period will apply and will expire SIX (6) MONTHS from the mailing date of this communication.
- Failure to reply within the set or extended period for reply will, by statute, cause the application to become ABANDONED (35 U.S.C. § 133). Any reply received by the Office later than three months after the mailing date of this communication, even if timely filed, may reduce any earned patent term adjustment. See 37 CFR 1.704(b).

**Status**

- 1) ☒ Responsive to communication(s) filed on 09 April 2004.
- 2a) ☐ This action is **FINAL**. 2b) ☒ This action is non-final.
- 3) ☐ Since this application is in condition for allowance except for formal matters, prosecution as to the merits is closed in accordance with the practice under *Ex parte Quayle*, 1935 C.D. 11, 453 O.G. 213.

**Disposition of Claims**

- 4) ☒ Claim(s) 1-18 and 25-72 is/are pending in the application.
- 4a) Of the above claim(s) \_\_\_\_\_ is/are withdrawn from consideration.
- 5) ☐ Claim(s) \_\_\_\_\_ is/are allowed.
- 6) ☐ Claim(s) \_\_\_\_\_ is/are rejected.
- 7) ☐ Claim(s) \_\_\_\_\_ is/are objected to.
- 8) ☒ Claim(s) 1-18 and 25-72 are subject to restriction and/or election requirement.

**Application Papers**

- 9) ☐ The specification is objected to by the Examiner.
- 10) ☐ The drawing(s) filed on \_\_\_\_\_ is/are: a) ☐ accepted or b) ☐ objected to by the Examiner.  
Applicant may not request that any objection to the drawing(s) be held in abeyance. See 37 CFR 1.85(a).  
Replacement drawing sheet(s) including the correction is required if the drawing(s) is objected to. See 37 CFR 1.121(d).
- 11) ☐ The oath or declaration is objected to by the Examiner. Note the attached Office Action or form PTO-152.

**Priority under 35 U.S.C. § 119**

- 12) ☐ Acknowledgment is made of a claim for foreign priority under 35 U.S.C. § 119(a)-(d) or (f).
- a) ☐ All b) ☐ Some \* c) ☐ None of:
1. ☐ Certified copies of the priority documents have been received.
2. ☐ Certified copies of the priority documents have been received in Application No. \_\_\_\_\_.
3. ☐ Copies of the certified copies of the priority documents have been received in this National Stage application from the International Bureau (PCT Rule 17.2(a)).
- \* See the attached detailed Office action for a list of the certified copies not received.

**Attachment(s)**

- 1) ☐ Notice of References Cited (PTO-892)
- 2) ☐ Notice of Draftsperson's Patent Drawing Review (PTO-948)
- 3) ☐ Information Disclosure Statement(s) (PTO-1449 or PTO/SB/08)  
Paper No(s)/Mail Date \_\_\_\_\_
- 4) ☐ Interview Summary (PTO-413)  
Paper No(s)/Mail Date. \_\_\_\_\_
- 5) ☐ Notice of Informal Patent Application (PTO-152)
- 6) ☐ Other: \_\_\_\_\_

## **DETAILED ACTION**

### ***Election/Restrictions***

Restriction to one of the following inventions is required under 35 U.S.C. 121:

- I. Claims 1-18, 25-31, 33, 35-36, drawn to a method for designing a metal ion for use in a molecular dynamics simulation, classified in class 703, subclass 11. If this Group is chosen, then the below mentioned species elections are also required.
- II. Claims 37-72, drawn to a machine for designing a metal ion for use in a molecular dynamics simulation, classified in class 703, subclass 11. If this Group is chosen, then the below mentioned species elections are also required.

Claims 32 and 34 are dependent from cancelled claims and are not considered in this restriction requirement. Upon amendment to proper dependent form, they may be considered.

The inventions are distinct, each from the other because of the following reasons:

Inventions I and II are unrelated. Inventions are unrelated if it can be shown that they are not disclosed as capable of use together and they have different modes of operation, different functions, or different effects (MPEP § 806.04, MPEP § 808.01). In the instant case the different inventions have different functions. While the invention of Group I is limited to one dummy atom, the invention of Group II can have multiple

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dummy atoms. The differences in the numbers of dummy atoms and other parameters make the two inventions distinct and provides undue search burden if searched together.

Because these inventions are distinct for the reasons given above and the search required for Group I is not required for Group II, restriction for examination purposes as indicated is proper.

***Species Elections for Group I:***

The applicant must choose a single specie from each of the below mentioned categories.

Category #1: Method of use of designing a metal ion.

Specie A: Method is used for a computer-aided protein-ligand docking simulation.

(Claim 4)

Specie B: Method is used for an energy refinement. (Claim 5)

Specie C: Method is used for simulating the charge-transfer effect of a transition metal ion. (Claim 6)

Generic to #1: Claims 1-3, 7-18, 25-31, 33, 35-36

Justification: Each method is a unique, distinct method of using the molecular dynamics simulation. Docking, energy refinements, and electrostatic effects are independent means of analyzing a simulation. The searches for each of the above terms are non-exclusive.

Category #2: Type of metal element to be used.

Applicant must choose not only if a transition metal (claims 7, 17, and 30) or a main group metal is to be employed (claim 8), but he must also determine which element is to be utilized of the lists in Claim 9, 10, 11, 12, 18, 29, and 31.

Generic to #2: Claims 1-6, 9-16, 25-28, 33, 35-36

Justification: Each type of metal ion requires its own search since each has its own intrinsic electrostatic, docking, and energetic properties. A search on all would provide undue burden. The searches for each of the above terms are non-exclusive.

Category #3: Type of use for the method of the base claim given an orientational requirement.

Specie D: Method is effective for maintaining said polyhedron geometry of said metal ion in organic and inorganic molecules in a nanosecond or longer MD simulation.  
(Claim 14)

Specie E: Method is effective for use in a computer-aided protein-ligand docking simulation. (Claim 15)

Specie F: Method is effective for use in a computer aided energy refinement. (Claim 16)

Specie G: Method is effective for simulating charge transfer effects of transition metal ions. (Claim 17)

Generic to #3: 1-13, 18, 25-31, 33, 35-36

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Justification: Each method is a unique, distinct method of using the molecular dynamics simulation. Docking, energy refinements, transition metal effects, and electrostatic effects are independent means of analyzing a simulation. The searches for each of the above terms are non-exclusive.

Category #4: Ranges of charge for the dummy atom.

Specie H: The dummy atom charge ranges between about +0.1 to about +3. (Claim 25)

Specie I: The dummy atom charge is about +0.5. (Claim 26)

Specie J: The dummy atom charge is about +0.3333. (Claim 27)

Generic to #4: Claims 1-18, 28-31, 33, 35-36

Justification: Each charge or ranges of charges imposes its own sets of limitations on the invention each of which is distinct and imposes its own additional search burden.

The searches for each of the above terms are non-exclusive.

### ***Species Elections for Group II:***

The applicant must choose a single specie from each of the below mentioned categories.

Category #1: Mass of the dummy atom

Specie K: mass equals about 0.1 g/mol (Claims 38, 56)

Specie L: mass is greater than about 0.1 g/mol (Claims 39, 57)

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Generic to #1: Claims 37, 40-55, 58-72

Justification: Each restriction on molecular mass is unique, distinct and imposes different requirements on molecular properties of the dummy atom. The searches for each of the above terms are non-exclusive.

Category #2: Shape of the polyhedron

The applicant must choose a shape of the polyhedron listed in claims 42, 43, 60, and 61. Each polyhedron type is a specific shape with differing geometric and as a result, molecular properties. The searches for each of the above shapes are non-exclusive

Generic to #2: Claims 37-41, 44-59, 62-72.

Category #3: Type of metal ion to be employed

Applicant must choose not only if a transition metal or a main group metal is to be employed (claims 44, 62), but he must also determine which element is to be utilized of the lists in Claim 45, 46, 48, 49, 62, 63, 64, 66, 67

Generic to #3: Claims 37-44, 50-61, 68-72

Justification: Each type of metal ion requires its own search since each has its own intrinsic electrostatic, docking, and energetic properties. A search on all would provide undue burden. The searches for each of the above terms are non-exclusive.

Category #4: Ranges of charge for the dummy atom.

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Specie M: The dummy atom charge ranges between about +0.1 to about +3. (Claim 52, 70)

Specie N: The dummy atom charge is about +0.5. (Claim 53, 71)

Specie O: The dummy atom charge is about +0.3333. (Claim 54, 72)

Generic to #4: Claims 37-51, 55-69

Justification: Each charge or ranges of charges imposes its own sets of limitations on the invention each of which is distinct and imposes its own additional search burden.

The searches for each of the above terms are non-exclusive.

Applicant is required under 35 U.S.C. 121 to elect a single disclosed species for prosecution on the merits to which the claims shall be restricted if no generic claim is finally held to be allowable.

Applicant is advised that a reply to this requirement must include an identification of the species that is elected consonant with this requirement, and a listing of all claims readable thereon, including any claims subsequently added. An argument that a claim is allowable or that all claims are generic is considered nonresponsive unless accompanied by an election.

Upon the allowance of a generic claim, applicant will be entitled to consideration of claims to additional species which are written in dependent form or otherwise include all the limitations of an allowed generic claim as provided by 37 CFR 1.141. If claims are added after the election, applicant must indicate which are readable upon the elected species. MPEP § 809.02(a).



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Should applicant traverse on the ground that the species are not patentably distinct, applicant should submit evidence or identify such evidence now of record showing the species to be obvious variants or clearly admit on the record that this is the case. In either instance, if the examiner finds one of the inventions unpatentable over the prior art, the evidence or admission may be used in a rejection under 35 U.S.C. 103(a) of the other invention.

Because these inventions are distinct for the reasons given above and have acquired a separate status in the art because of their recognized divergent subject matter, restriction for examination purposes as indicated is proper.

Applicant is advised that the reply to this requirement to be complete must include an election of the invention to be examined even though the requirement be traversed (37 CFR 1.143).

Papers related to this application may be submitted to Technical Center 1600 by facsimile transmission. Papers should be faxed to Technical Center 1600 via the central PTO Fax Center. The faxing of such pages must conform with the notices published in the Official Gazette, 1096 OG 30 (November 15, 1988), 1156 OG 61 (November 16, 1993), and 1157 OG 94 (December 28, 1993)(See 37 CFR § 1.6(d)). The Central PTO Fax Center Number is (571) 273-8300.

Any inquiry concerning this communication or earlier communications from the examiner should be directed to Russell Negin, Ph.D., whose telephone number is (571) 272-1083. The examiner can normally be reached on Monday-Friday from 7am to 4pm.

If attempts to reach the examiner by telephone are unsuccessful, the examiner's Supervisor, Ardin Marschel, Ph.D., Supervisory Patent Examiner, can be reached at (571) 272-0718.

Any inquiry of a general nature or relating to the status of this application should be directed to Legal Instrument Examiner, Tina Plunkett, whose telephone number is (571) 272-0549.

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Information regarding the status of the application may be obtained from the Patent Application Information Retrieval (PAIR) system. Status information for published applications may be obtained from either Private PAIR or Public PAIR. Status information for unpublished applications is available through Private PAIR only. For more information on the PAIR system, contact the Electronic Business Center (EBC) at 866-217-9197 (toll-free).

-RSN 12/19/05

*RAA 12/19/05*

*John S. Brusca 20 December 2005*

**JOHN S. BRUSCA, PH.D  
PRIMARY EXAMINER**